ALS Users Meeting, October 20, 2004

Resonant Inelastic X-Ray Scattering and Soft X-Ray Emission studies of Electronic Structure in Thin Film Organic Semiconductors.

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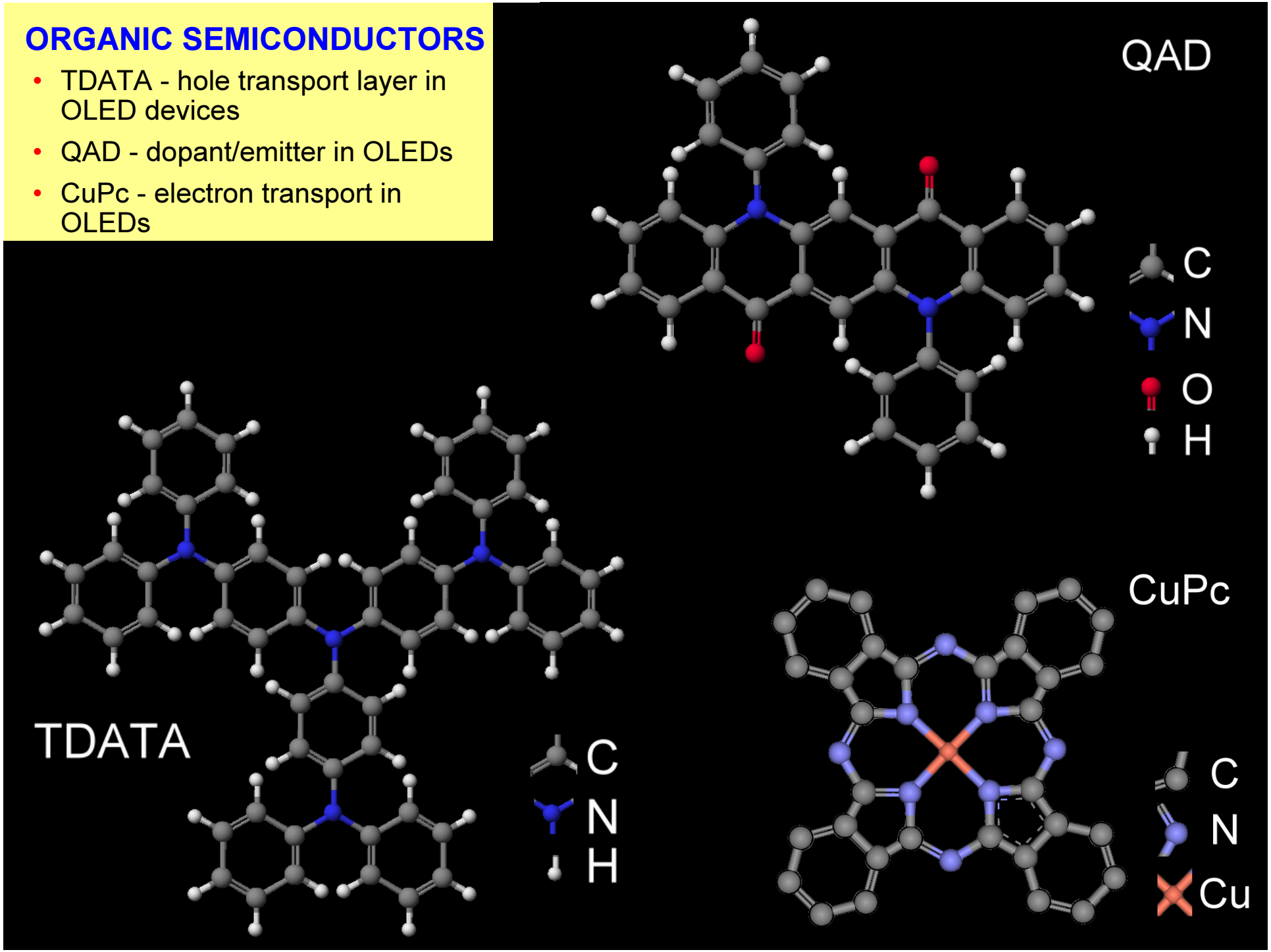
- Experiments performed at the NSLS on beamline X1B

Motivation

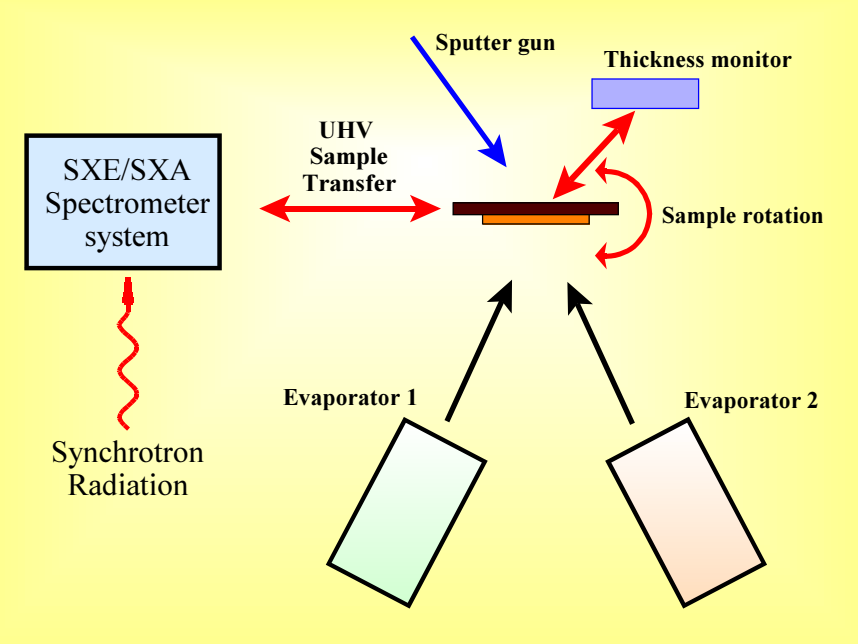
- There is significant technological interest in the development of carbon-based electronic devices.
- Numerous organic compounds are being used and/or studied as electronic materials.
- Detailed synchrotron-based spectroscopic measurements of their electronic structure are generally lacking.
- Photoemission is less than ideal in this regard due to the fact that the photoemission process leaves the organic system in an ionized state.
- Resonant soft x-ray emission holds the promise of accurate and detailed electronic structure measurement.

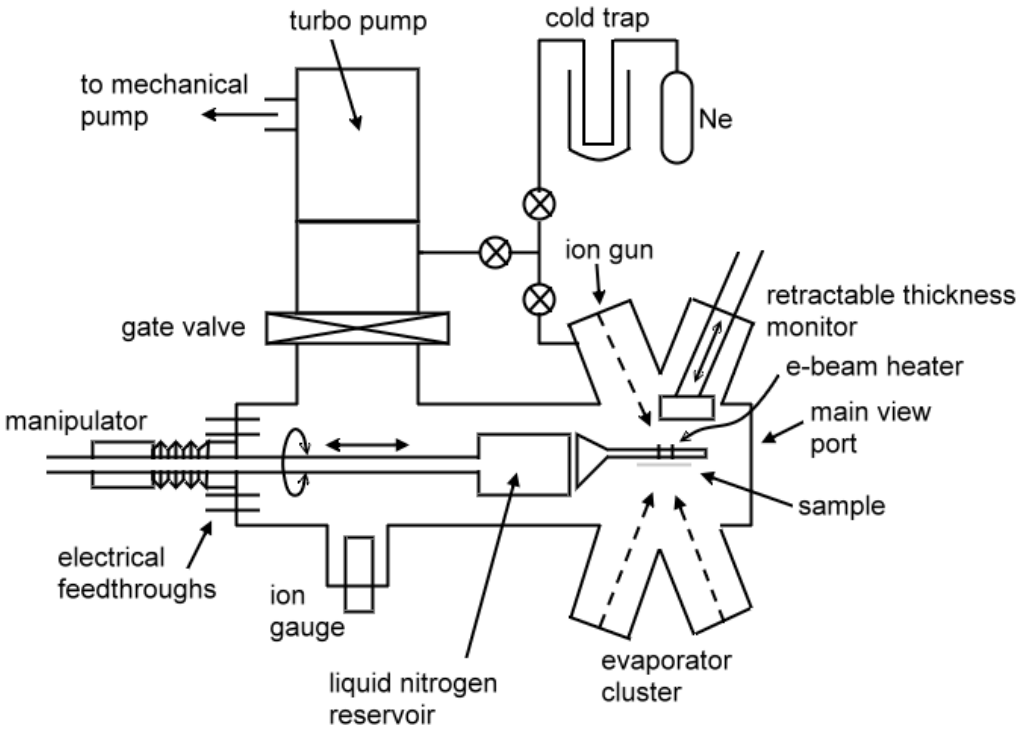
ORGANIC SEMICONDUCTORS

- TDATA - hole transport layer in OLED devices
- QAD - dopant/emitter in OLEDs
- CuPc - electron transport in OLEDs



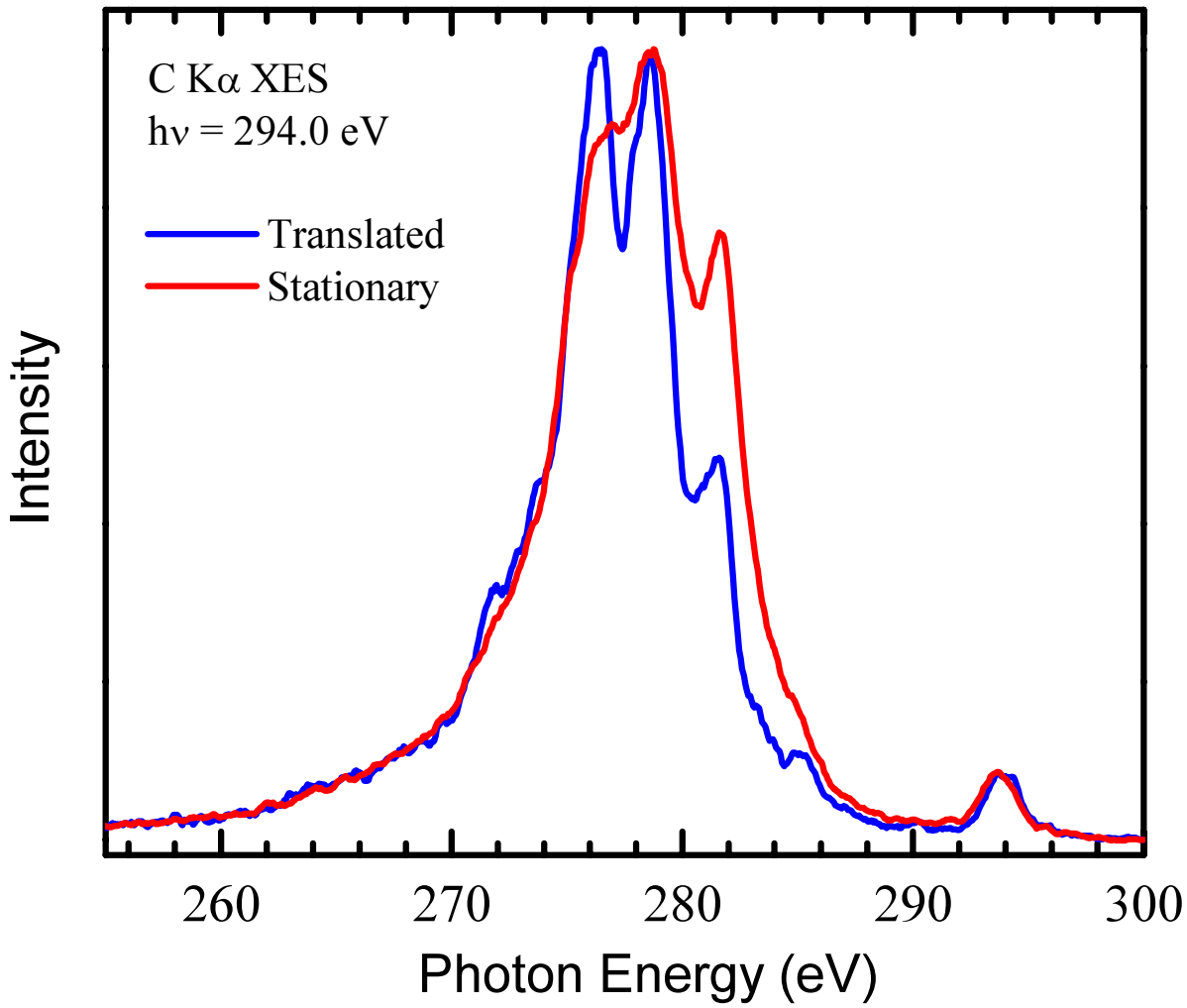
Compact UHV System for Organic Molecular Beam Deposition (OMBD)

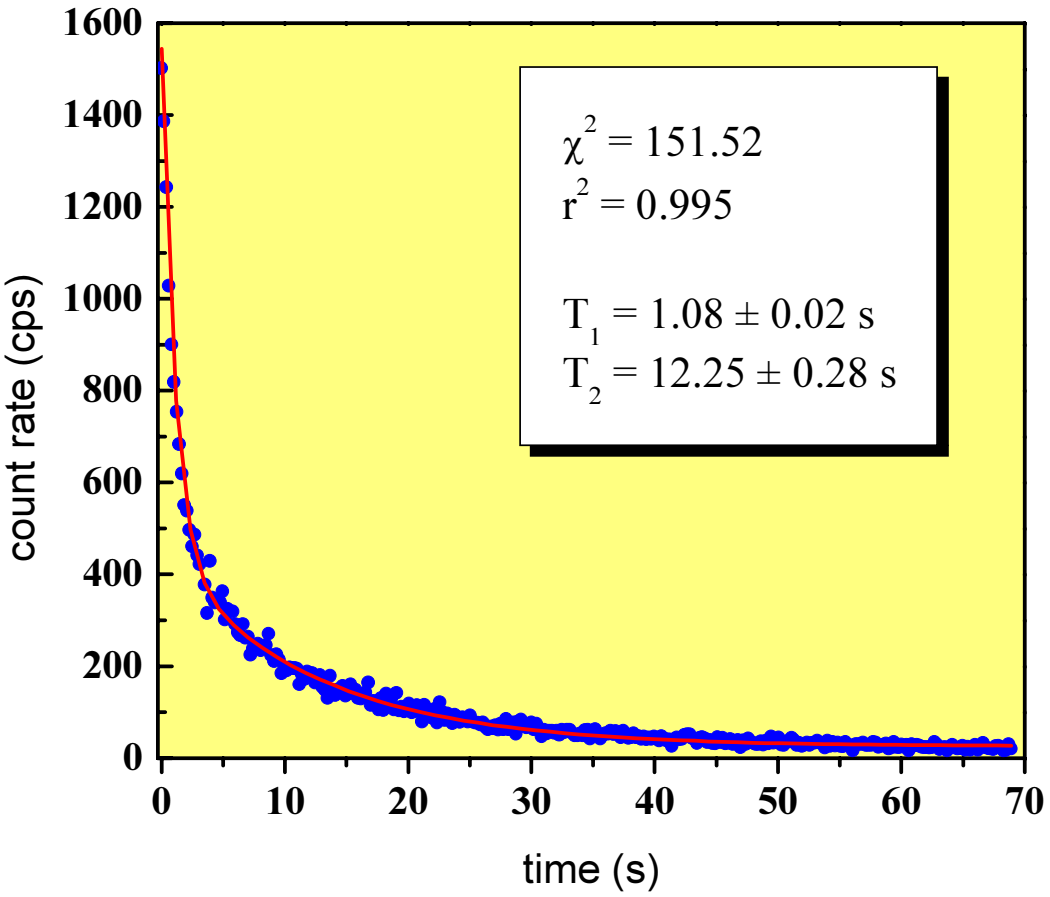




- Custom UHV system attached directly to the main measurement system to allow in-situ growth and characterization. Pressure ~1x10^{-9} torr.
- Provides:
  - 3 or 4 organic evaporators.
  - Quartz thickness monitor.
  - Inert gas ion gun + gas manifold system.
  - Sample heating & cooling - 100K-1000K.
  - Sample load-lock.

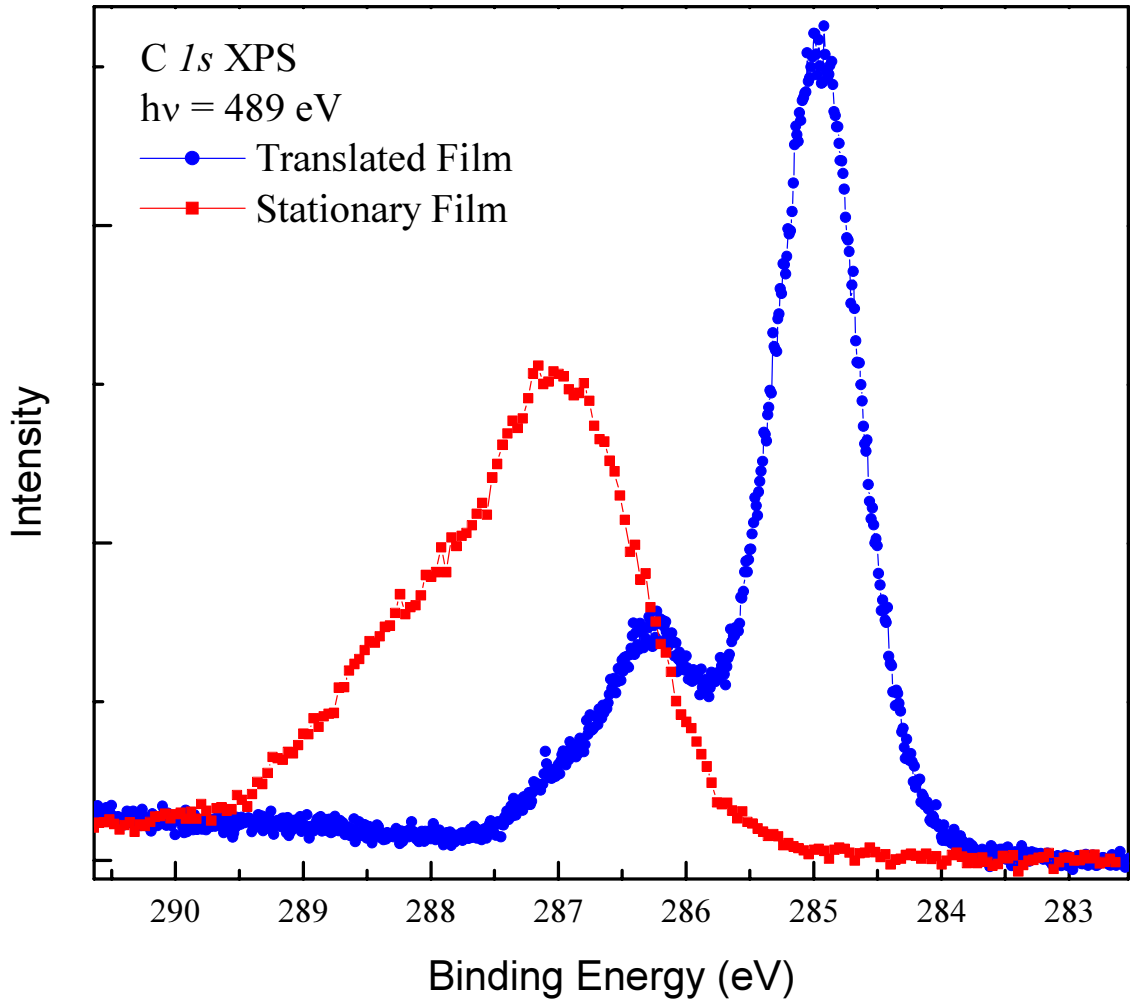
SXE from CuPc - Translated vs. Stationary samples





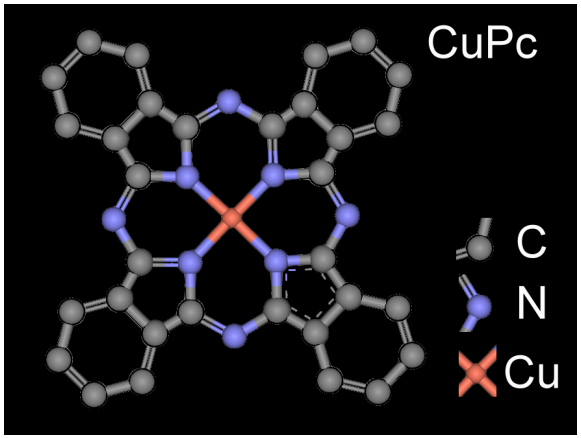
Decay of the intensity of elastic scattering of 286.3 eV photons from $(ET)_2SF_5CH_2CF_2SO_3$-type film

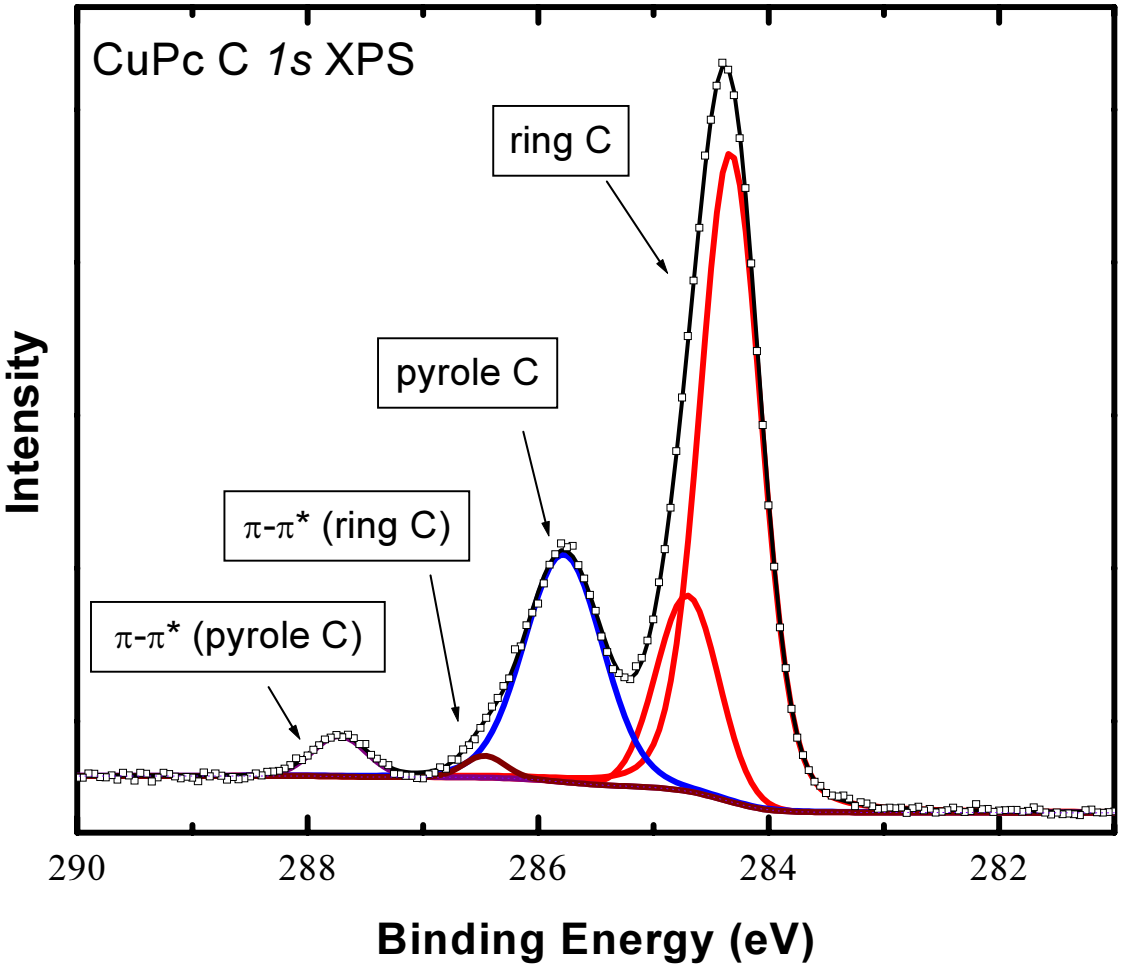
Core Level Photoemission of C *1s* States in QAD Films

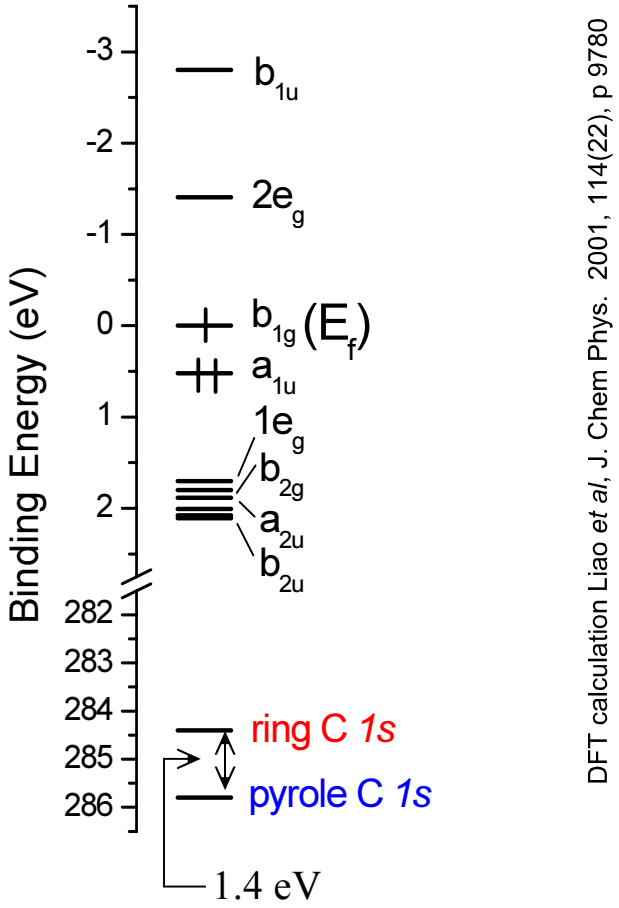


Copper phthalocyanine Cu-Pc

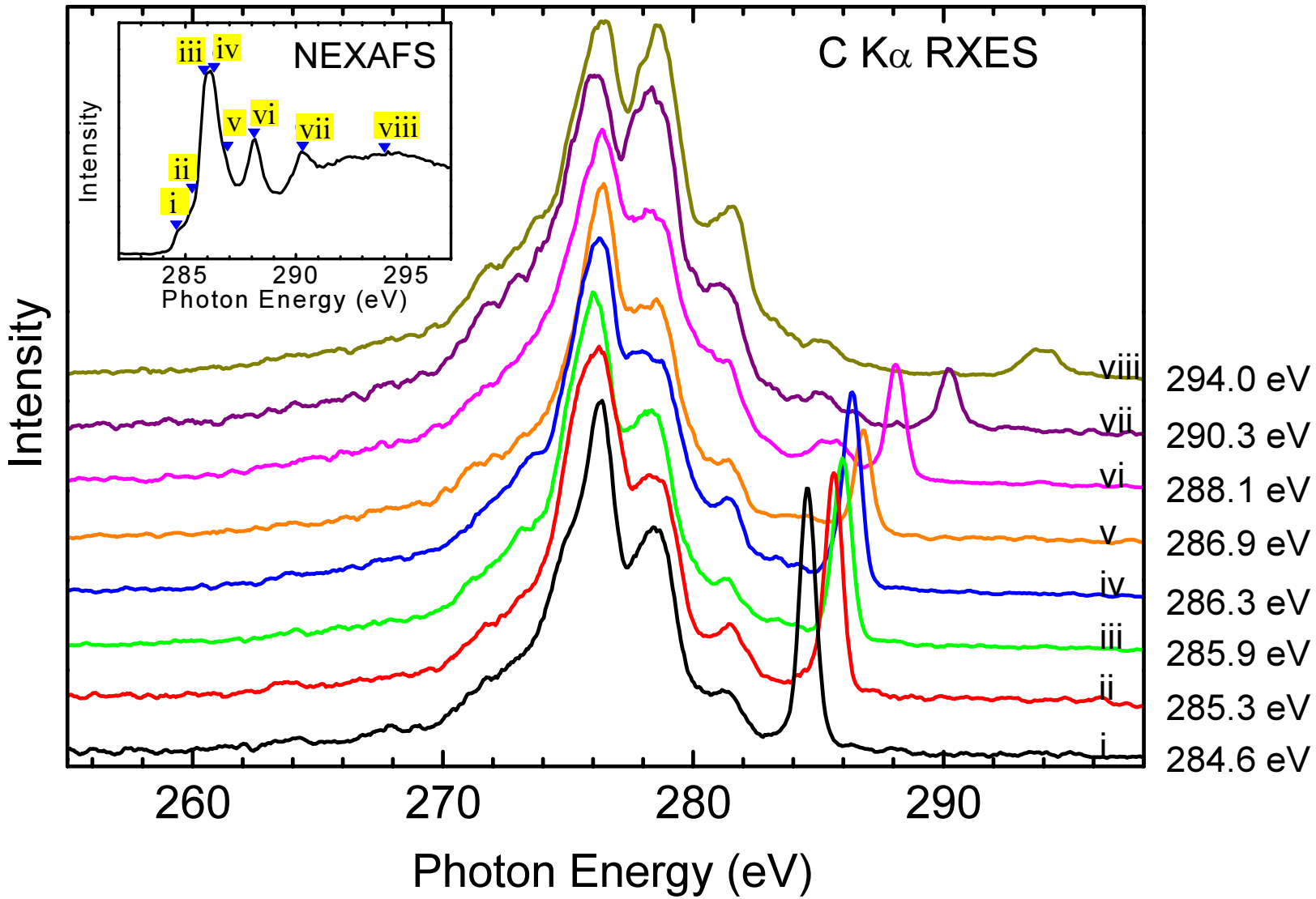
- Complex electronic structure
- Cu^{2+} ion - *3d* electrons hybridized with ligand (C,N) *2p* states



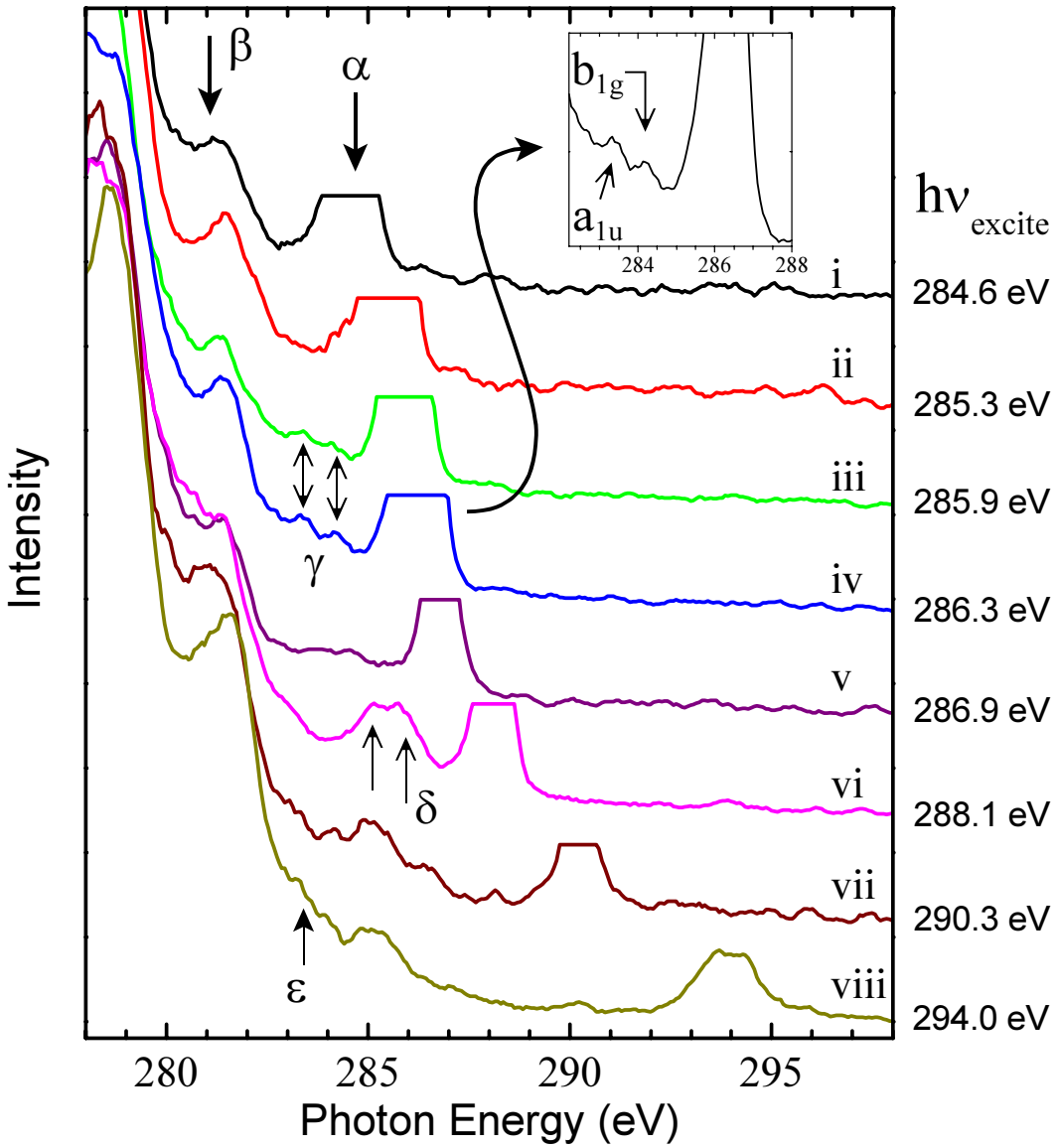


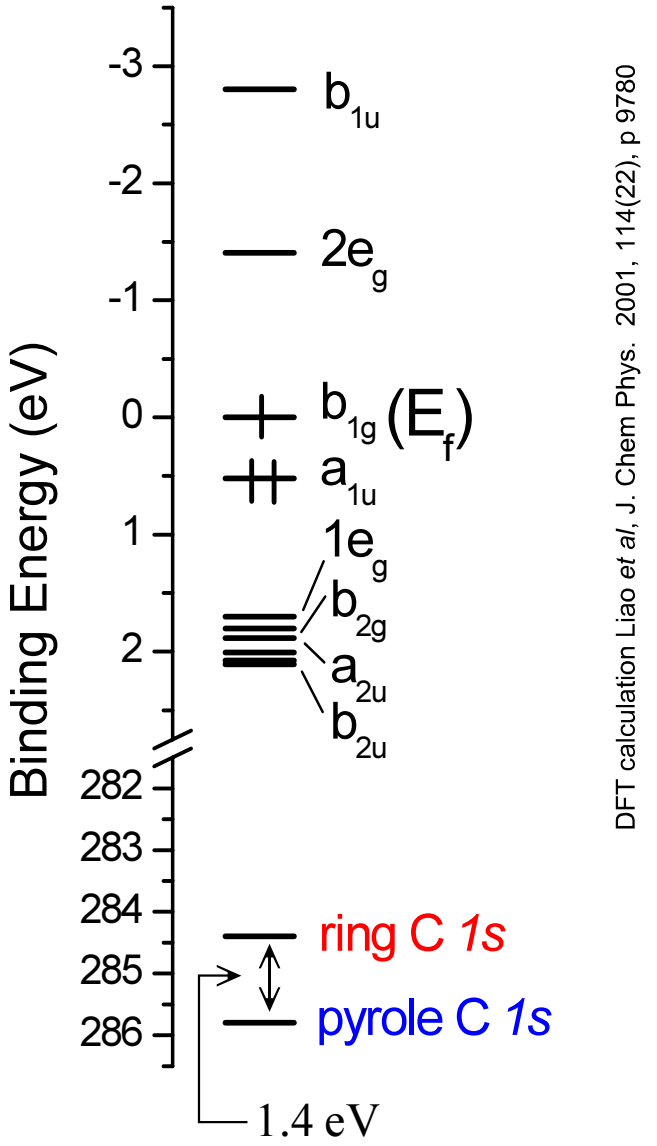


Copper phthalocyanine RXES



CuPc - RXES detail

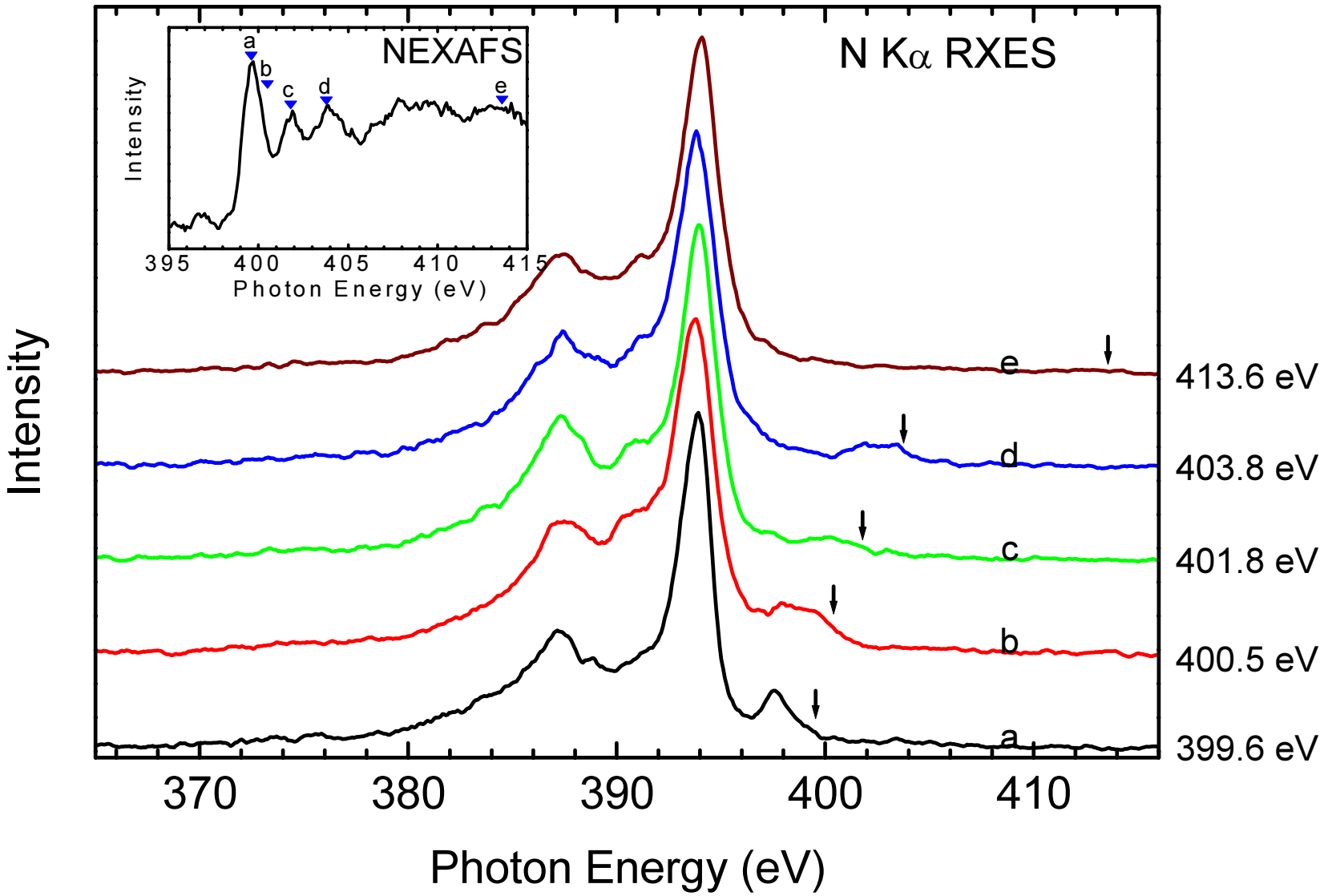




DFT calculation Liao *et al*, J. Chem Phys. 2001, 114(22), p 9780

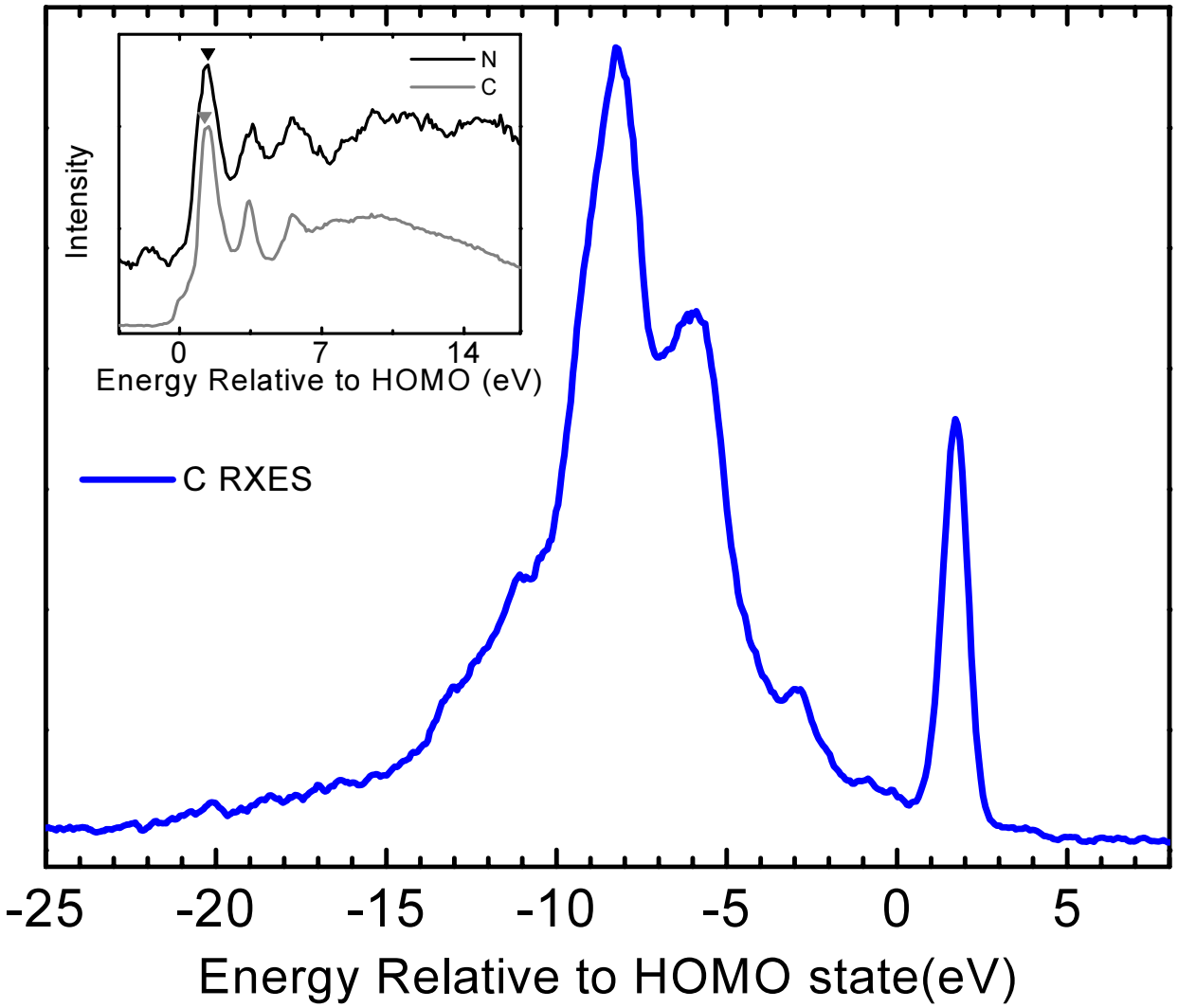
Copper phthalocyanine RXES

- Two N sites expected - only 0.4 eV separation



CuPc RXES / UPS comparison

- RXES represents *2p* character of C and N states of the valence band
- UPS represents joint or total density of states of the valence band



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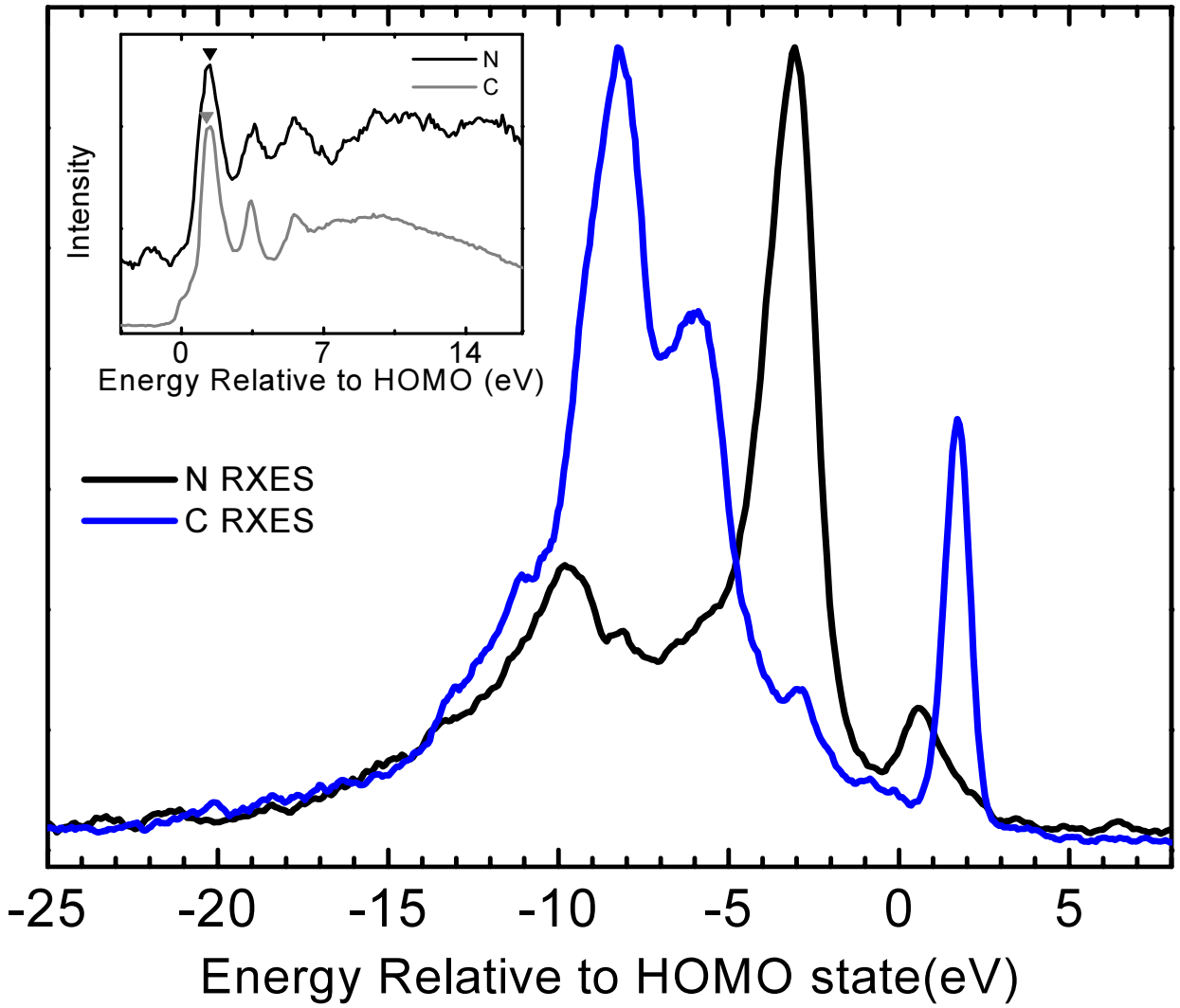

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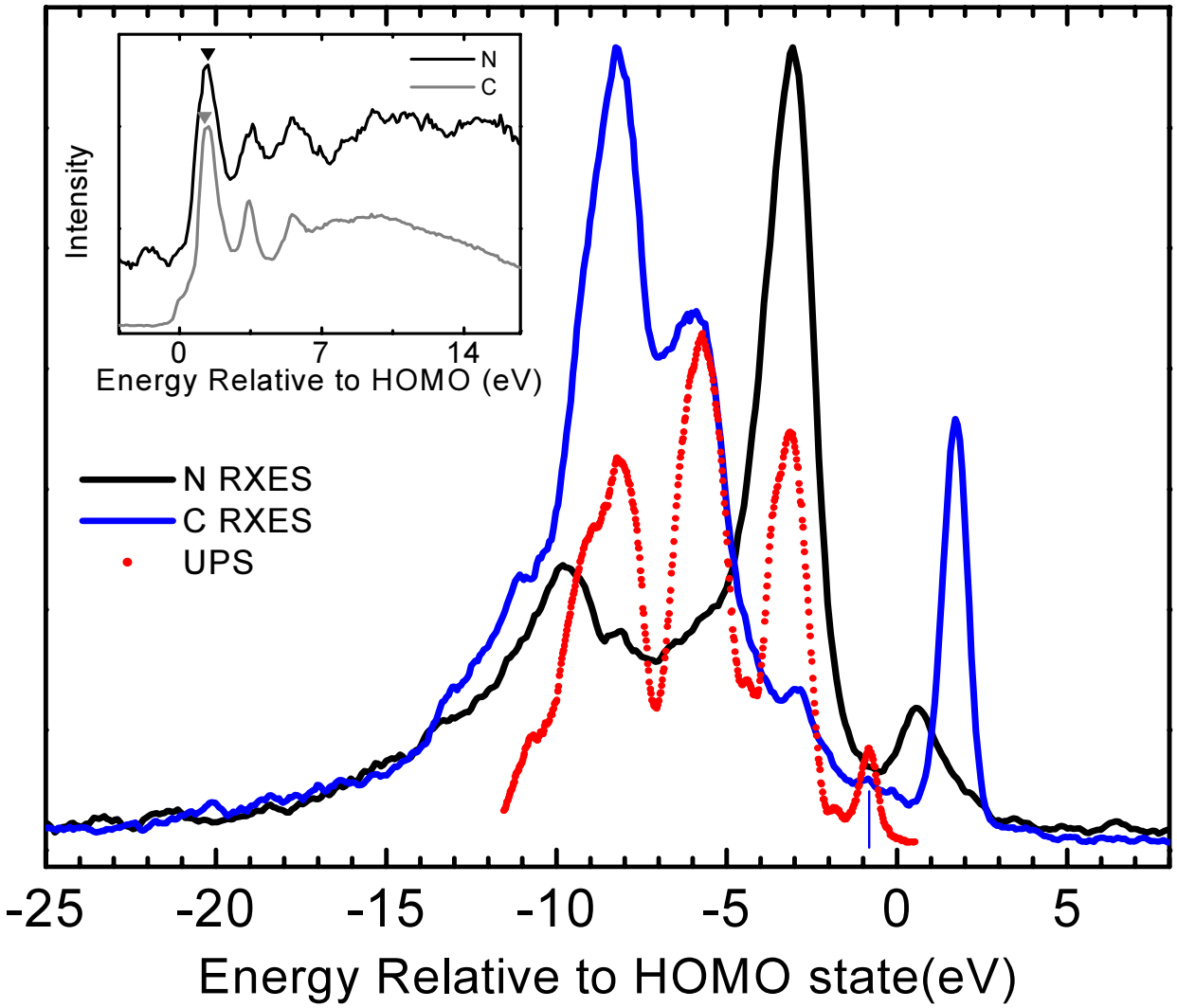

UPS from Chasse *et al*, J. Appl. Phys. 1999, **85**(9), p6589

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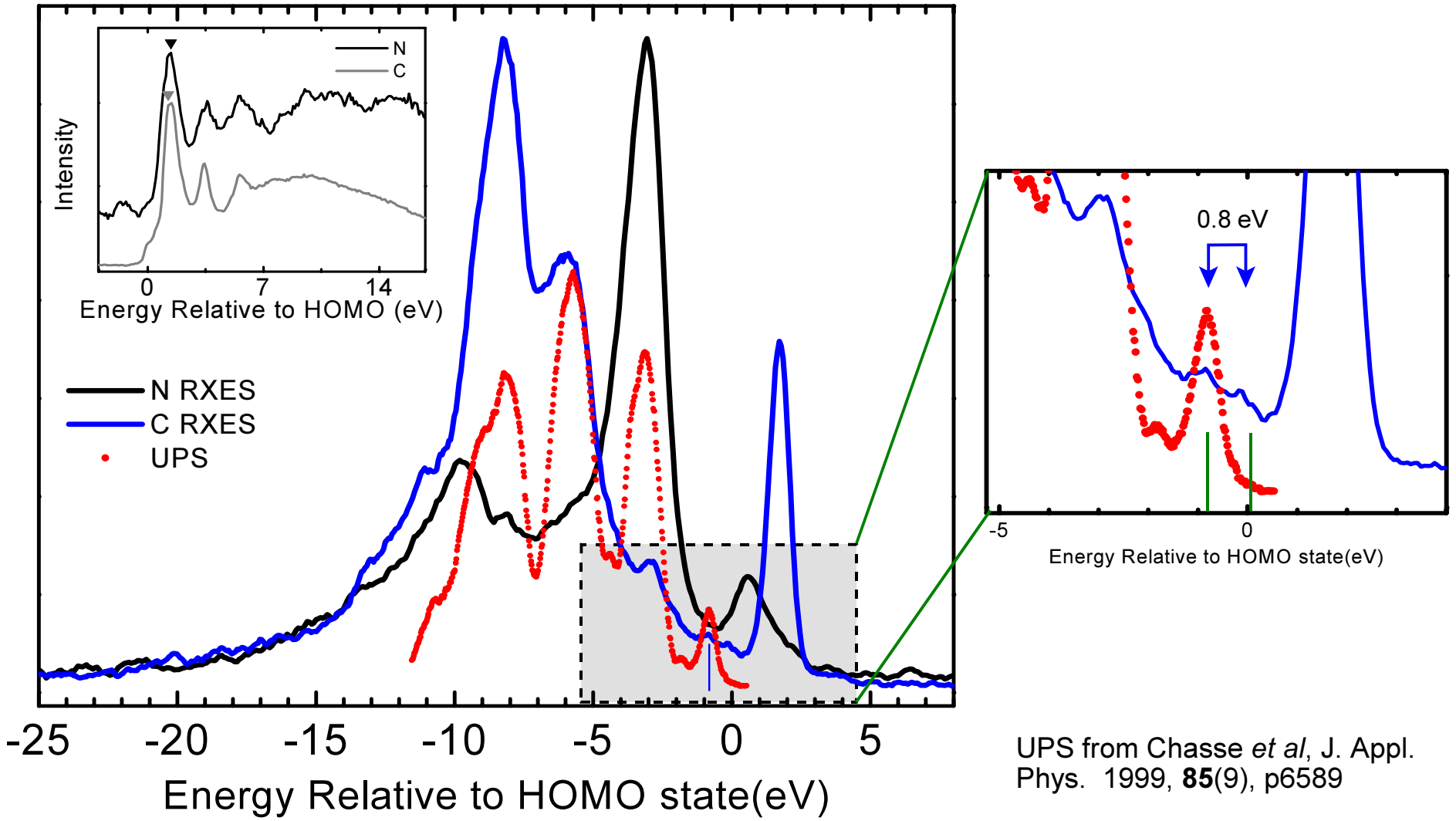
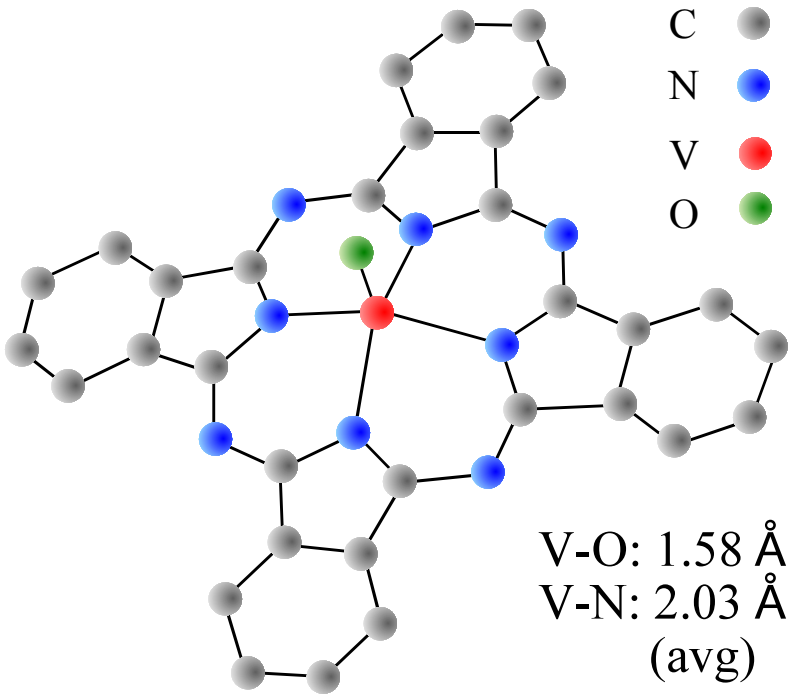
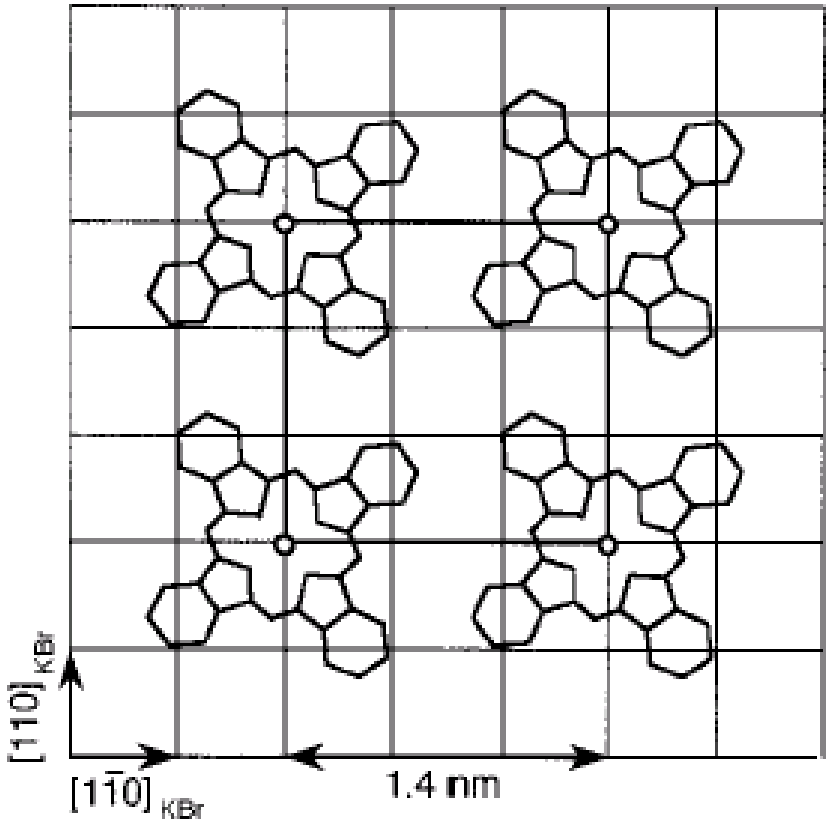


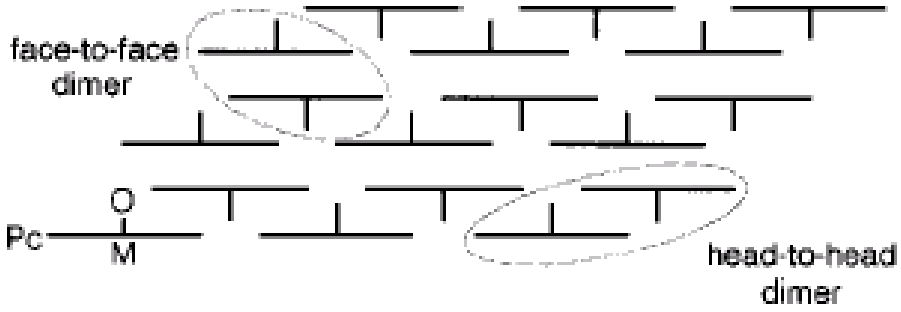
UPS from Chasse *et al*, J. Appl. Phys. 1999, **85**(9), p6589

VO-Pc thin film structure



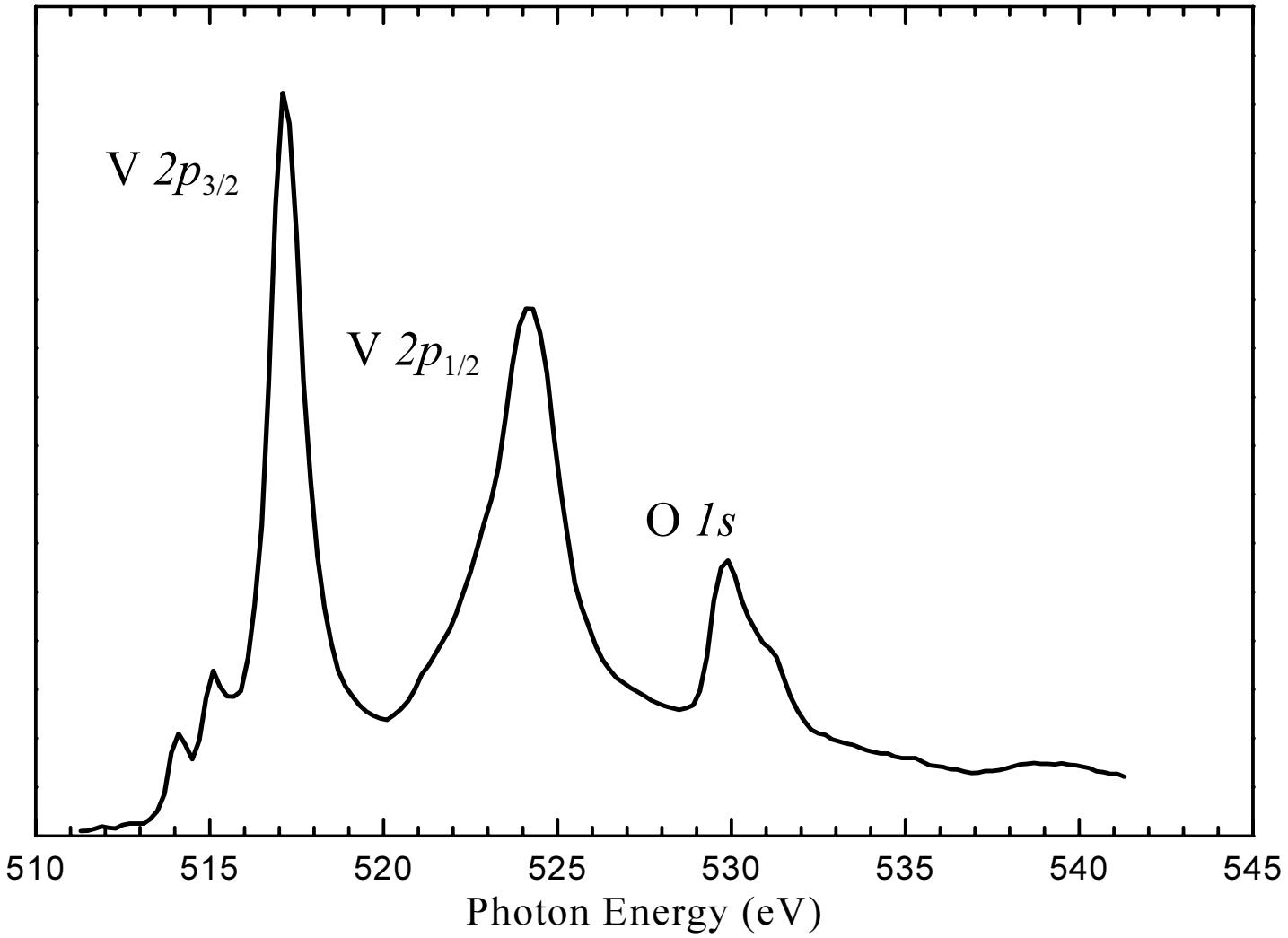
V-O: 1.58 Å
V-N: 2.03 Å
(avg)



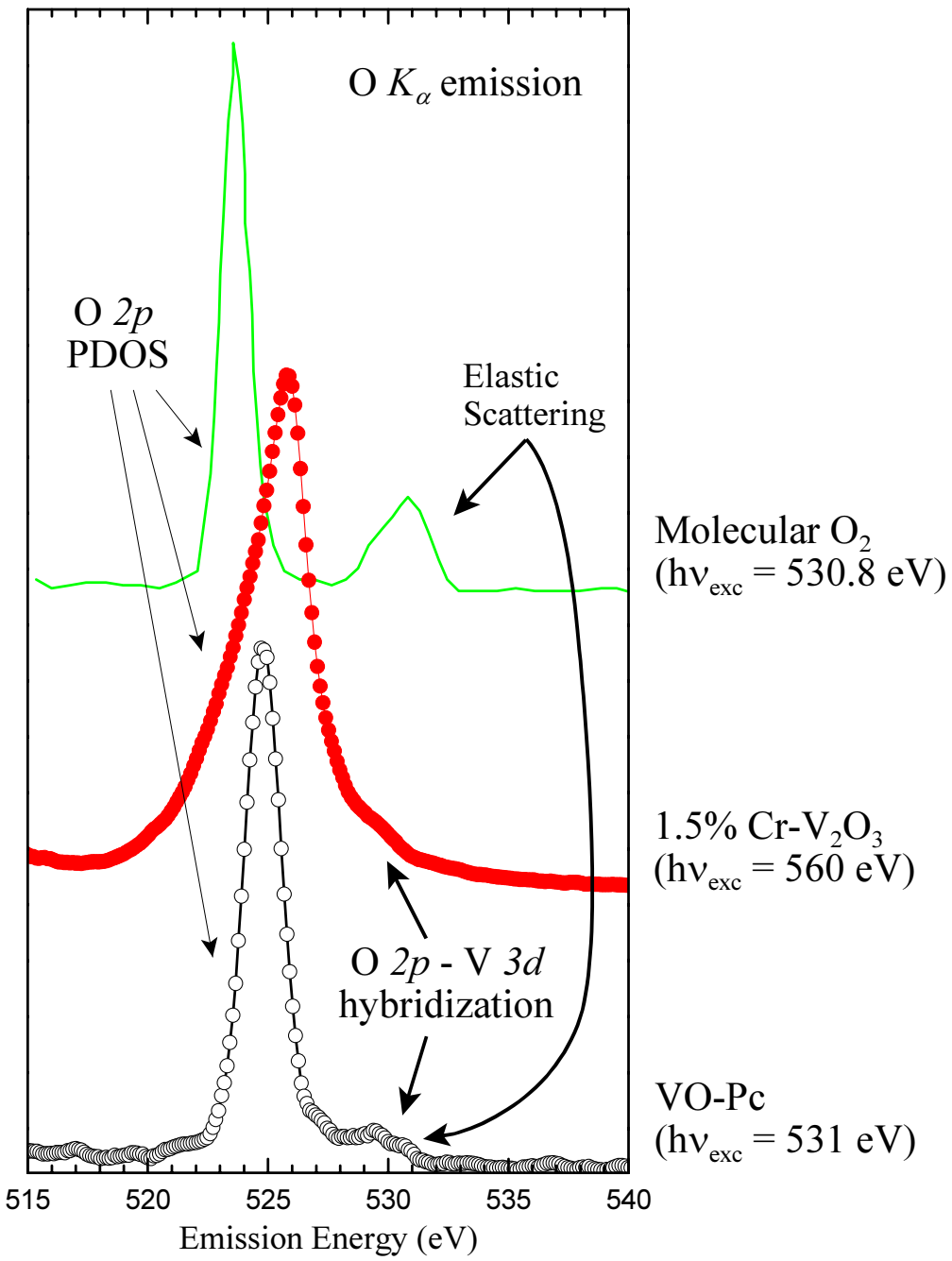


Yanagi *et al*, J. Appl. Phys. **81**, 7306 (1997)

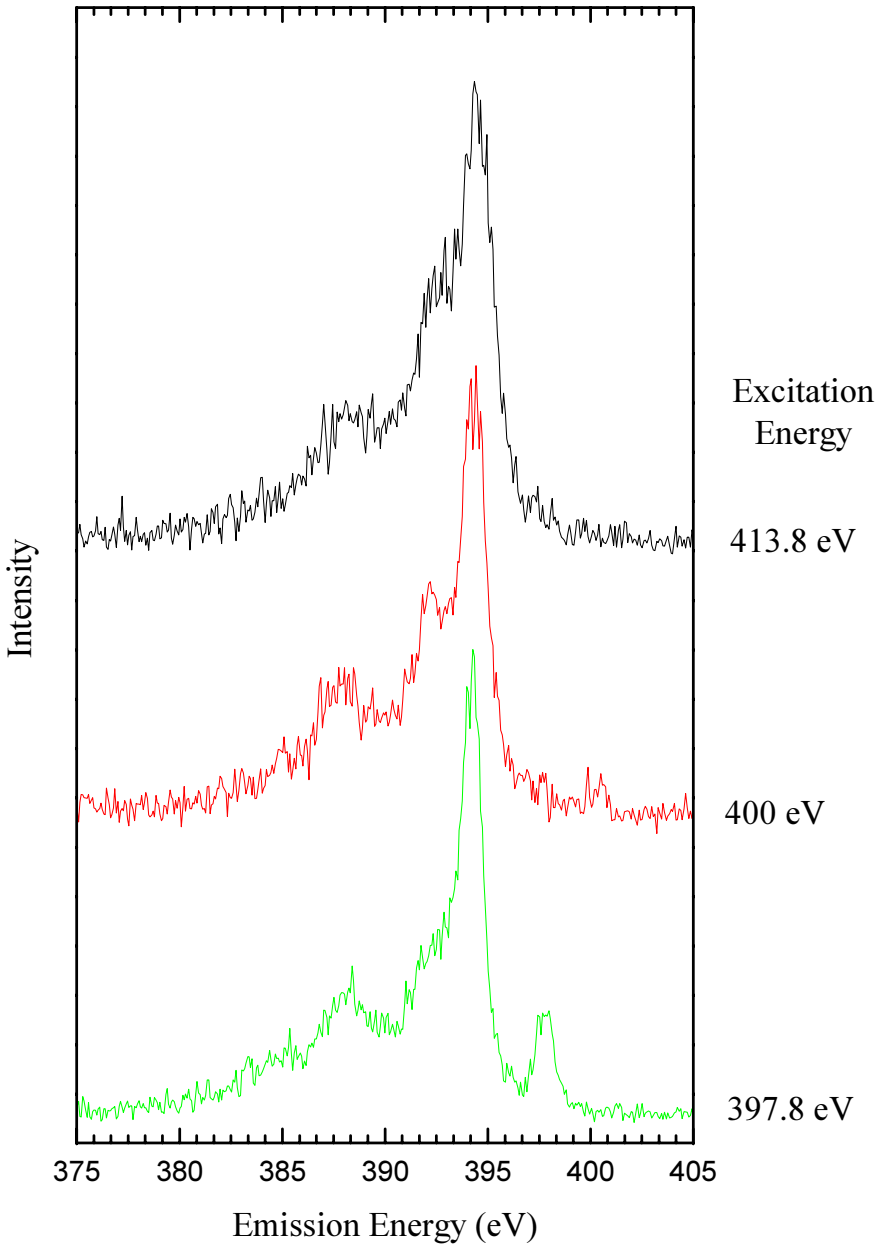
VO-Pc: V *2p* & O *1s* XAS



O 2p emission



N *2p* states in VO-Pc



Summary

- Spectroscopic studies of the electronic structure of organic solids must explicitly address beam damage.
- Thin films can be grown *in situ* by OMBD at synchrotron radiation sources.
- Continuous translation of large area thin films is a viable solution to beam damage issues
  - *Marked changes in the measured SXE and XPS spectra are observed between translated and stationary films.*
- Data presented for a variety of organic semiconductors: TDATA, QAD, CuPc.
- RSXE a powerful probe of non-ionized electronic structure.....